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Los Alamos NATIONAL LABORATORY

"Learning to navigate working within a nuclear facility, in addition to learning the basics of plutonium metallurgy, is a unique opportunity that keeps me interested and engaged."

Meghan Gibbs recognized with 2021 ASM Bronze Medal Award

Meghan Gibbs, a research and development engineer on the Materials Properties Team in Nuclear Materials Science (MST-16), has been recognized with the 2021 ASM Bronze Medal Award, awarded by ASM International, the world's largest materials science and engineering society. ASM International cited Gibbs for "excellence in process modeling, manufacturing science, and professional service impacting the U.S. steel industry and product qualification for the U.S. Nuclear Deterrent."

Challenging and complicated work

The society's highly competitive Bronze Medal—only two were awarded—recognizes ASM members who are in early-career positions for their significant contributions in the field of materials science and engineering through technical content and service to ASM and the materials science profession.

As part of the Materials Properties Team since joining the Laboratory in 2015, Gibbs studies plutonium casting process modeling, mold design, and process development in support of manufacturing and science programs. A self-described "jack of all trades" who straddles the line between science and manufacturing, Gibbs is also interested in plutonium thermophysical properties and plutonium aging studies, using differential scanning calorimetry and density to contribute to a variety of scientific programs.

"Plutonium is a really challenging, complicated material," Gibbs said, "especially when you add in constraints that are unlike most materials research—safety and security are two that are at the forefront. Learning to navigate working within a nuclear facility, in addition to learning the basics of plutonium metallurgy, is a unique opportunity that keeps me interested and engaged. Casting is the first step in producing everything from research samples to manufactured parts."

That casting work relies heavily on modeling and simulation. Gibbs has learned advanced programs such as Truchas, a simulation tool for casting developed under the Advanced Simulation and Computing Program. Her experience with hands-on manufacturing—she worked as a control metallurgist at an ArcelorMittal steel plant in Indiana before joining the Lab—means she appreciates what the virtual R&D processes can mean for working with materials.

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From Ellen's desk . . .

> *As we begin the new fiscal year, I think now is a good time to reflect on some of the incredible accomplishments and changes within the division this year."*

Dear MST,

As we begin the new fiscal year, I think now is a good time to reflect on some of the incredible accomplishments and changes within the division this year. I will start by talking about some of the obvious changes in MST leadership. Over the course of FY21, we welcomed Kim Defriend back to MST-7, as group leader, and Gary Gladysz back to Los Alamos National Laboratory as her deputy. This of course left a spot to fill in MST-8 and again, there we were able to welcome Kurt Sickafus back to Los Alamos as group leader. In June, Jon Bridgewater joined ALDWP, as a subject matter expert, to help with challenges associated with the Laboratory's 30 pits per year mission, and with that began a search for a new deputy division leader. While that search is not yet complete—we are getting close. I want to personally thank ALDWP and MST-16 for "lending" the division office Bob Putnam and Matt Jackson to serve in that role. Additionally, special thanks to David Moore for serving as acting group leader in Matt's absence.

I am also proud of some of the facility and capability changes we (MST) have enabled this year. As a division we grew by 55 FTEs this year—which represents a tremendous amount of hiring, when one considers attrition. Our budget also grew, by approximately $15 million, and this along with our staffing growth is driving a careful look at how we use our existing facilities as well as what we will need in the future. With that said, folks in MST-7 have been doing hard work to examine space utilization. This has led to clean out of labs, expansion of the vault, and expansion of drop-in space for staff who work in a hybrid fashion. MST-16 has finished REI-2 and is very close to realizing Hazard Categorization 3 in the RLUOB. This is a project that has been decades in the making. This past year, MST-8 notably received Congressional approval for the Low Enriched Fuel Fabrication Facility to begin construction at TA-35 and oversaw important electrical upgrades in the Ion Beam Materials Lab. Finally, MST-DO, partnering with Sigma, MPA, and ALDPS, is examining plans for the future materials campus at TA-3. These plans are just beginning and the division office is eager to share them with you once we have a clearer sense of how to realize that vision.

We also have had a large number of technical and programmatic accomplishments this year, which I hope to highlight in detail at our All Hands later this month. Here, I will identify just a few. MST-7 hosted ALDW and ALDX offices to showcase new technologies in polymer synthesis for the W93. This is complemented by MST-7 being selected as the home for the new program manager for the Advanced Engineering Materials Program. Additionally, MST-7 has been expanding its additive manufacturing capabilities and, notably, just received and installed a new selective laser sintering platform in support of the additive coordination team efforts across the NNSA. MST-16 ended the year having authored two highly visible, Level Two milestones for the Office of Experimental Sciences and having played key roles in realizing completion of an aggressive schedule of Pu surveillance tests—reported directly to NA-10—as well as in addressing challenges associated with our 30 pits a year mission through the use of advanced metallography capabilities. Finally, I am thrilled that MST-8 has had its scientific excellence recognized this year in two particularly notable ways: (1) the selection of Stuart Maloy as ANS Fellow and (2) the selection of Blas Uberuaga as Laboratory Fellow. Congratulations Stu and Blas!

As we start the new fiscal year, we will certainly be looking forward to more changes and growth. In the meantime, I hope that you can join the division office on October 14 for our division All Hands meeting, where we plan to celebrate these and a much broader set of achievements from this past year.

Stay safe,

Ellen

Gibbs cont.

“When we’re talking about how to cast plutonium, if we can model the system and vary parameters via simulations, we can work to minimize the number of experiments we have to do in real life, reducing development time and hopefully understanding the process a little bit more,” Gibbs said. “This brings a lot of cost savings and value to the programs.”

A value on service and education

Gibbs was nominated by ASM International’s Los Alamos chapter, where she has held several leadership positions. The chapter offers awards and scholarships to local high school and college students, takes part in science fairs, and has participated in STEM programs at the high school.

Gibbs will receive the Bronze Medal at IMAT 2022, the International Materials Applications & Technologies Conference and Exhibition, the society’s annual meeting.

Technical contact: Meghan Gibbs ■

Rodgers awarded DOE NNSA graduate fellowship

Colorado School of Mines graduate student Brian Rodgers is set to take advantage of the experimental science opportunities available at Los Alamos National Laboratory beginning this fall.

As a recipient of a DOE NNSA Laboratory Residency Graduate Fellowship (LRGF), Rodgers will work with Saryu Fensin, Dynamic and Quasi-Static Loading (experimental) Team leader in Materials Science in Radiation and Dynamics Extremes (MST-8). Rodgers will perform molecular dynamics simulations augmented by machine learning to determine the solid-liquid interfacial energy of aluminum-silver of different crystallographic orientations with varying alloy compositions.

Experimental methods to measure the interfacial energy of a solid and a liquid of the same composition are difficult to perform and prone to error. Molecular dynamics can determine this material parameter but require time, expertise, and powerful computers, all of which are available at Los Alamos. During his fellowship, which consists of a minimum of two 12-week periods, Rodgers will perform the simulations and design and implement experiments to validate the results.

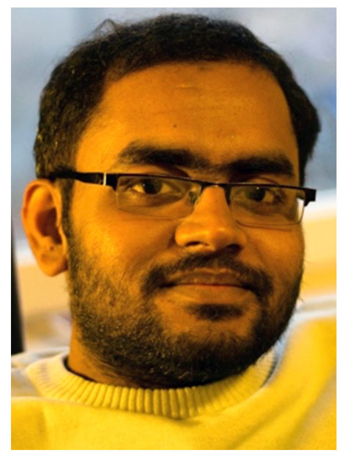
While this information is crucial to understanding and predicting the microstructures developed during solidification in this particular alloy, this project sets the stage in development of a toolkit that can be used to predict processing-structure relationships, a key goal within the manufacturing area of leadership for LANL.

Rodgers, who earned his MS in metallurgical and materials engineering in 2019, is due to receive his PhD in spring 2023. His research aims to develop a deeper understanding of solidification behavior and microstructural development during additive manufacturing.

Launched in 2017, the LRGF program connects students pursuing PhDs in fields of study that address complex science and engineering problems critical to stewardship science with scientists at DOE NNSA facilities.

Technical contact: Saryu Fensin ■

Banerjee accepted to RSC; named outstanding peer reviewer



Amitava Banerjee (Materials Science in Radiation and Dynamics Extremes, MST-8) has been admitted as a Royal Society of Chemistry (RSC) associate member and named a top reviewer of its *Journal of Materials Chemistry A*.

Of the more than 51,000 active peer reviewers assessing manuscripts for the weekly journal, only 500 are recognized each year based on the number, timeliness, and quality of the reports they completed over the last year. The weekly journal focuses on novel materials related to energy and sustainability.

A Director’s Postdoctoral Fellow, Banerjee studies defect thermodynamics and kinetics pertaining to corrosion mechanisms as part of the MST-8 Radiation Science Modeling Team. His work examines the complexity of the metal/oxide interface in a variety of contexts, which is important for designing and tailoring composite materials properties for various applications.

Banerjee earned his Master of Technology in materials science and engineering from the Indian Institute of Technology in Kanpur, India, and his PhD in energy conversion and storage from Uppsala University in Sweden.

Technical contact: Amitava Banerjee ■

Beaux earns early career award for innovative research

Miles Beaux (Engineered Materials, MST-7) is among 83 scientists who will receive a total of $100 million through the DOE Early Career Awards Program, which supports critical research at universities and national laboratories.

The DOE program supports exceptional scientists working in the agency's priority research areas. For example, Beaux's work has established plutonium capabilities for scanning probe microscopy that do not exist anywhere else, according to MST-7 Group Leader Kimberly DeFriend.

"These capabilities contribute to the Lab's larger mission by providing a means to seamlessly probe density of states of neptunium, plutonium, and americium. Beaux's hypotheses attempt to explain the complexity and properties of actinide materials," she said.

"Winning this award is a great honor, and brings a sense of validation to the establishment of a scanning tunneling microscopy capability for plutonium research," Beaux said. "By performing scanning tunneling spectroscopy on a range of bulk single crystal actinide intermetallic compounds, a seamless mapping of both the occupied and unoccupied electronic structures of these materials can be obtained using a local probe, providing a means by which their complex chemical and physical properties can be understood."

Beaux joined the Laboratory in 2010. His expertise in applying photoemission spectroscopy techniques to actinide materials earned him a Seaborg Postdoctoral Fellowship. In 2012 Beaux served as chief technology officer for a startup company called MJ3 Industries, LLC. He returned to Los Alamos in 2014 and has authored or co-authored 10 scholarly publications. Beaux's work supports the Lab's Stockpile Stewardship mission area and the Materials for the Future science pillar.

Technical contact: Miles Beaux

Euser recognized for Science in '3' presentation

Ginny Euser (Materials Science in Radiation and Dynamics Extremes, MST-8) was recognized as an outstanding presenter in the Lab's Science in "3" event.

In the career development event organized by the Postdoc Program Office, Laboratory postdoctoral researchers present their research for a general audience in three minutes or less, challenging the postdoc to give a clear and concise presentation.

Euser's presentation "The need for speed: Measuring friction at high sliding velocities," described an experimental fixture designed to enable friction measurements across a wide range of sliding velocities to ultimately inform friction models used in simulations of dynamic processes. The novel experimental setup Euser introduced will aid in the fundamental understanding of interfacial friction, as well as provide a framework for generating friction data to validate existing friction models.

Euser is a postdoctoral research associate in MST-8's Dynamic and Quasi-Static Loading Team. She joined LANL in February 2020 and works primarily on a Laboratory Directed Research and Development-Exploratory Research project focused on exploring the effect of sliding velocity on interfacial friction. She is mentored by Ben Morrow (MST-8) and Nicholas Denissen (XTD Primary Physics, XTD-PRI). She has a PhD from the Colorado School of Mines in metallurgical and materials engineering.

Technical contact: Ginny Euser

Uberuaga named LANL Fellow

Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MT-8) has been named a 2021 Los Alamos National Laboratory Fellow.

"To be a Fellow at the Laboratory is to be a leader in our workplace and within the scientific community at large," said Lab Director Thom Mason.

For more than 20 years, Uberuaga has contributed to the field of atomistic modeling of radiation effects in materials where he performed pioneering research in complex oxides and nanomaterials. He is the director of DOE's Fundamental Understanding of Transport Under Reactor Extremes (FUTURE), which researches the extreme conditions of irradiation and corrosion that impact materials in nuclear reactors. His scientific work to understand these effects continues to showcase the Laboratory's expertise. Additionally, he's shown exceptional leadership in the mentoring of 27 postdoctoral researchers and 6 graduate students.

Technical contact: Blas Uberuaga

Machine learning aids discovery of new double perovskite oxides

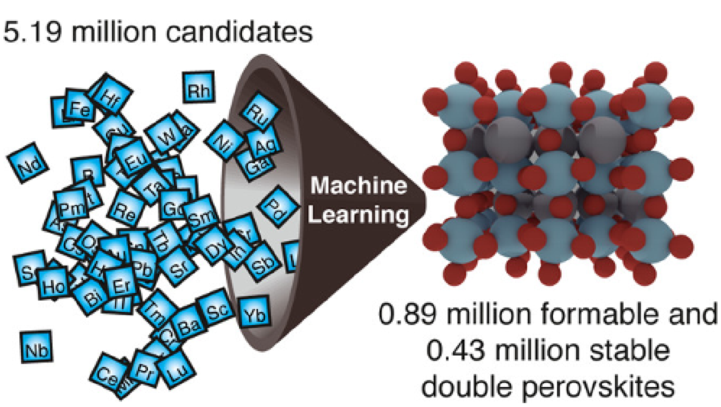
Technique is first step toward systematically identifying materials designed for advanced applications

Perovskite oxides continue to attract interest due to their fascinating and wide-ranging properties for diverse applications. The tunability of these properties may be further enhanced by increasing their compositional complexity via double perovskite-ordered configurations containing multiple cations.

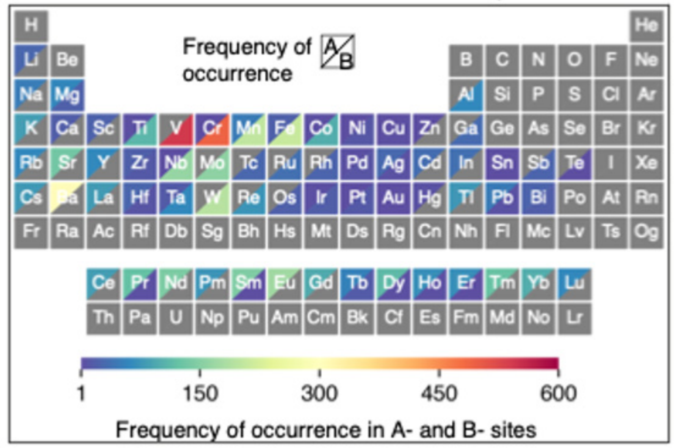
In work featured in *Chemistry of Materials,* Los Alamos materials scientists applied machine learning and first principles computations in tandem to explore an exhaustive chemical space of single and double oxide perovskites. Demonstrating the utility of its machine learning approach, the team identified more than 400,000 likely stable compositions with 414 that are particularly promising candidates for future experimental synthesis of novel oxide perovskites. Their work significantly extends the chemical space of known perovskites that can be considered for a range of applications.

More generally, the study highlights the potential for using machine-learning-guided high-throughput calculations to identify novel chemistries that may exhibit enhanced functionality. Thus, it serves as the first step in a more comprehensive research plan in which the functionality of promising compounds is examined, opening new avenues for materials designed for new and novel applications.

The team examined the relationship between formability—the practical ability to synthesize a compound—and stability—the thermodynamic preference to form the structure. Formability and stability training data sets were developed using existing experimental literature and in-house density functional theory computations, containing 1,505 and 3,469 examples, respectively, which represents state of the art in the current open literature in perovskite and double perovskite compounds. Subsequently, cross validated and highly accurate machine learning classification models were built using these training data sets and employed to screen for novel stable oxide perovskites.



The study identifies (1) atomic features relevant to predicting formability and stability in perovskite and double perovskite compounds, (2) the importance of including energy contributions due to local structural relaxations going beyond the high symmetry perovskite phase, and (3) 437,828 double perovskite compounds that are likely to be stable and 891,188 compounds that are likely to be formable.



The machine learning approach identified 414 novel cubic double perovskite chemistries spanning the periodic table with high confidence.

The Laboratory Directed Research and Development Program funded the work, which supports the Lab's Energy Security mission and its Materials for the Future and Information Science and Technology science pillars. In particular, the team's machine learning approach is part of Los Alamos's efforts to develop advanced and new materials by intentionally controlling their functionality and predicting their performance—the key goal of the Lab's Materials for the Future strategy. The Lab's high performance computing clusters provided computational support.

Researchers: Anjana Talapatra, Blas P. Uberuaga, Christopher R. Stanek, and Ghanshyam Pilania (Materials Science in Radiation and Dynamics Extremes, MST-8). Reference: "A machine learning approach for the prediction of formability and thermodynamic stability of single and double perovskite oxides," *Chemistry of Materials* (2021).

Technical contact: Anjana Talapatra

Measuring sub-surface corrosion in plutonium storage containers

Researchers at Los Alamos National Laboratory, Savannah River National Laboratory (SRNL), and other DOE sites are working to better understand corrosion in stainless steel storage containers used to store excess plutonium-bearing materials. A Los Alamos team has developed an imaging technique to assess sub-surface cracks in containers for the first time and begin to predict the lifetime of the container—crucial information for ensuring the safe storage of plutonium materials.

continued on next page

Measuring sub-surface cont.

Plutonium is packaged across the entire DOE Complex in 3013 containers designed to safely store plutonium metals and oxide for up to 50 years for use in future missions. Unfortunately, corrosion pits have been observed on the inside surface of the containers storing hydrated chloride-bearing plutonium. Surface microscopy can be used to measure the pits' depths, but provides no information about the sub-surface extent.

To measure the extent of sub-surface damage, a surveilled destructive examined (DE) 3013 container, previously packaged at Hanford with hydrated chloride-bearing plutonium oxide materials, was opened at SRNL and cut into several pieces for nondestructive 3D imaging using x-ray computed tomography. With this technique, 2D reconstructed slices and 3D renderings of not only the surface corrosion pits, but also the sub-surface cracks, are possible.

The samples were imaged at Los Alamos in Engineered Materials (MST-7) using the Versa 520 micro-x-ray computed tomography instrument to visualize the depth and amount of corrosion cracking with a ~2µm voxel size. Due to the potential contamination, the samples were kept double bagged and x-ray imaged in situ. Figure 1 is a reconstructed 3D image of three corrosion features along the inside surface of the container near the weld region. Figure 2 is a higher resolution image of one of the features. The renderings are inverted in that the steel is transparent and the surfaces and void space are rendered solid. Figure 3, a single reconstructed slice through the corrosion is shown. With these images, the researchers can measure the depth of the pits and the extent of the corrosion (~300µm for this one in particular).

This work was funded by the Material Identification and Surveillance (MIS) Program, led by LANL Program Manager Laura Worl (Pit Production Mission Integration, PPMI-DO), which supports the entire DOE Complex. The team included Juan G. Duque (Physical Chemistry and Applied Spectroscopy, C-PCS), Brian M. Patterson and Lindsey Kuettner (MST-7), Daniel Rios (Materials Recovery and Recycle, AMPP-4), and other members of the MIS team. Nuclear Materials Science (MST-16) provided transport and packaging support.

Technical contacts: Brian M. Patterson and Juan G. Duque

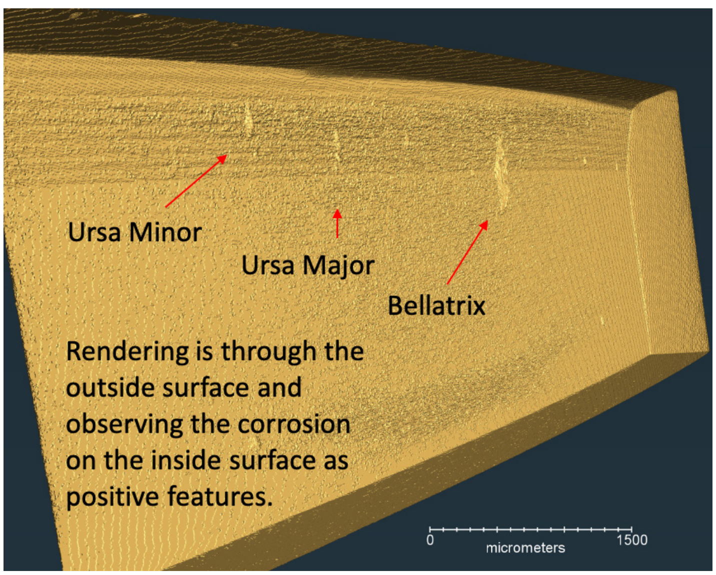


Figure 1: A reconstructed 3D image of three corrosion features along the inside surface of the container near the weld region. This image shows the three major features observed on the surface of one of the samples.

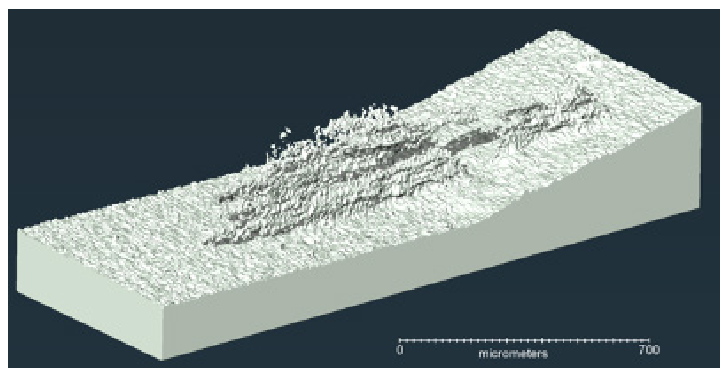


Figure 2: A high resolution inverted sub-surface image at Bellatrix. (The feature is rendered positive, in that the steel is transparent and the surfaces are rendered solid). This image shows the intricate corrosion ramifications within the sub-surface that cannot be seen on the surface image.

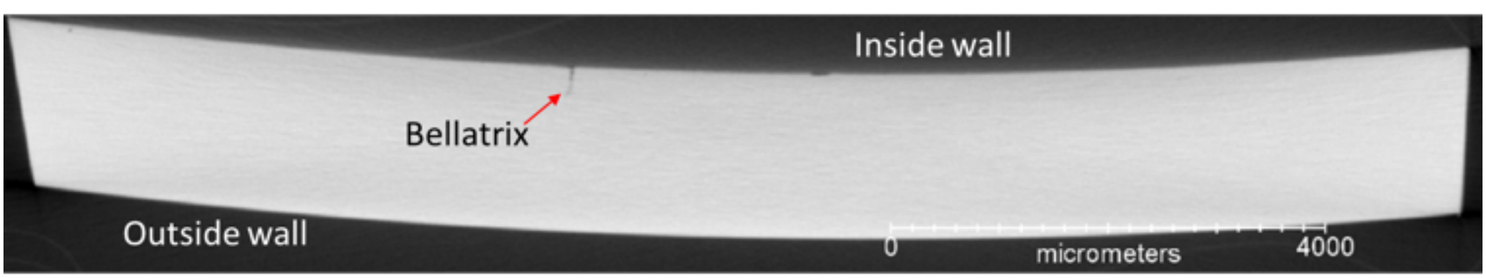


Figure 3: A single slice through the corrosion at Bellatrix. This image shows extent of the corrosion with features extending into the sub-surface for ~300µm.

Recognizing commitment to worker environment, safety, security

Congratulations to MST's FY21 WESST Star Award recipients.

- Kim Pestovich, MST-8
- Matthew Schneider, MST-8
- Michael Torrez, MST-8

Star Awards recognize badge-holding employees who put safety and security into everything they do.

Celebrating service

Congratulations to the following MST employees who recently celebrated service anniversaries.

Randall Randolph, MST-7 .... 35 years
Michael Ramos, MST-16 .... 25 years
Angelique Wall, MST-16 .... 25 years
Ellen Cerreta, MST-DO.. 20 years
Rachel Morse, MST-DO .... 20 years
John Martinez, MST-7 .... 15 years
Benjamin Eftink, MST-8... 10 years
Sarah Hernandez, MST-16....................................... 10 years
Benjamin Hollowell, MST-16.................................... 10 years
Benjamin Morrow, MST-8 .... 10 years
Joseph Torres, MST-7 .... 10 years
Carlos Archuleta, MST-16.. 5 years
Laurent Capolungo, MST-8 .... 5 years
Matthew Chancey, MST-8 .... 5 years
Kyle Cluff, MST-7... 5 years
Osman El Atwani, MST-8... 5 years
Cisco Gonzales, MST-8... 5 years
Alexander Long, MST-8... 5 years
Ramon Martinez, MST-8.. 5 years
Tomas Martinez, MST-16... 5 years
Paul Peterson, MST-7 .... 5 years
Todd Steckley, MST-16.. 5 years
Brenden Wiggins, MST-7... 5 years
Christopher Wilson, MST-7.. 5 years

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NNSA National Nuclear Security Administration

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Heads UP!

Preventing backing-up incidents

Operating a motor vehicle or heavy equipment is an inherently hazardous task, yet backing up a vehicle creates more risk for incidents to occur.

According to the Bureau of Labor Statistics, in 2019 there were 73 work fatalities where workers were killed by a vehicle backing up in a roadway, work zone, or parking lot. This does not include the number of fatalities that occur from backing-up incidents outside of work. According to the National Safety Council, backing-up incidents cause 500 deaths and 15,000 injuries per year. Therefore, it is important for all drivers and equipment operators to be aware of potential hazards to prevent work injuries or fatalities from happening.

Backing-up incidents occur because drivers cannot see a worker who is either standing, walking, or kneeling behind the vehicle/heavy equipment. The driver or equipment operator may not see the worker behind the vehicle because the worker might be in a blind spot, or the driver/equipment operator might assume the area is clear. Additionally, workers might not hear the vehicle/equipment's back-up alarms due to surrounding noise and not move out of the path of travel.

To prevent backing-up incidents/accidents from occurring, both the drivers/operators need to look out before backing up the vehicle, and workers need to look out before walking behind or near vehicles/heavy equipment.

The best way to prevent backing-up incidents and accidents is to eliminate backing up as much as possible and/or planning the vehicle/heavy equipment's movements before moving. Take these steps to create a safe environment:

- Look for pull-through parking before choosing where to park.
- Complete a walk around of the vehicle/heavy equipment prior to backing up so that you are aware of the path of travel.
- Use the vehicle's back-up cameras and proximity warning systems where possible, but do not be over-reliant on back-up cameras.
- Use spotters when necessary, but be aware that they may be at additional risk performing this function in busy spaces.

Backing up a vehicle or heavy equipment can almost always be eliminated or greatly reduced when proper planning is used. Eliminating having to back up should be the first choice before relying on less effective safeguards.